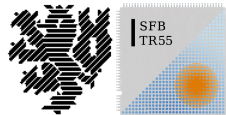# Ab initio calculations in lattice QCD

Z. Fodor

University of Wuppertal

what is the source of the mass of ordinary matter?

how and when was it generated?

(lattice theory talk: systematics)

SFB
TR55

# Outline

**1** Introduction

**2** Mass of the proton

**3** Finite temperature QCD transition

**4** Summary

## The origin of mass of the visible Universe

source of the mass for ordinary matter (not a dark matter talk)

basic goal of LHC (Large Hadron Collider, Geneva Switzerland):

"to clarify the origin of mass"

e.g. by finding the Higgs particle, or by alternative mechanisms
order of magnitudes: 27 km tunnel and 10 billion dollars

## The vast majority of the mass of ordinary matter

ultimate mechanism: responsible for the mass of the electron and for the mass of the quarks

interestingly enough: just a tiny fraction of the visible mass (such as stars, the earth, the audience, atoms)
electron: almost massless, $\approx 1/2000$ of the mass of a proton
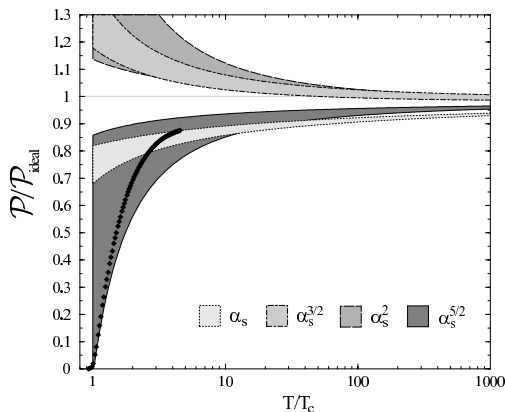quarks: also almost massless particles

the vast majority (about 95%) comes through another mechanism
$\Longrightarrow$ this mechanism and this 95% will be the main topic of this talk

(quantum chromodynamics, QCD) on the lattice

## QCD: need for a systematic non-perturbative method

in some cases: good perturbative convergence; in other cases: bad
pressure at high temperatures converges at $T=10^{300}$ MeV

## Degrees of freedom

even worse: no sign of the same physical content

Lagrangian contains massless gluons & almost massless quarks
we detect none of them, they are confined
we detect instead composite particles: protons, pions

proton is several hundred times heavier than the quarks
              how and when was the mass generated

qualitative picture (contains many essential features):
in the early universe/heavy ion experiment: very high temperatures
(motion)
it is diluted by the expansion (of the universe/experimental setup)
small fraction remained with us confined in protons
$\Rightarrow$ the kinetic energy inside the proton gives the mass ($E = mc^2$)

## Lattice field theory

systematic non-perturbative approach (numerical solution):

<div align="center">quantum fields on the lattice</div>

quantum theory: path integral formulation

quantum mechanics: for all possible paths add exp(iS)
quantum fields: for all possible field configurations add exp(iS)

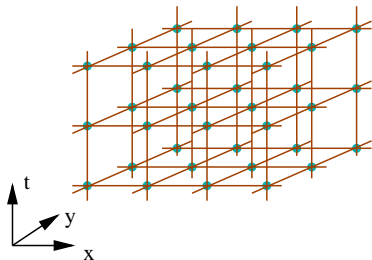Euclidean space-time (t=$i\tau$): exp(-S) sum of Boltzmann factors

we do not have infinitely large computers $\Rightarrow$ two consequences

a. put it on a space-time grid (proper approach: asymptotic freedom)
formally: four-dimensional statistical system
b. finite size of the system (can be also controlled)

$\Rightarrow$ polynomial problem, with reasonable size/spacing: solvable

fine lattice to resolve the
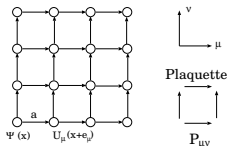structure of the proton ($\lesssim$0.1 fm)
few fm size is needed

thermodynamics: $T=1/(aN_t)$ at a fixed T
reducing "a" means increasing $N_t$

mathematically
$10^9$ dimensional integrals

advanced techniques,
good balance and
several Tflops are needed

# Lattice Lagrangian: gauge fields



$$\mathcal{L} = -\tfrac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar{\psi}(D_\mu \gamma^\mu + m)\psi$$

anti-commuting $\psi(x)$ quark fields live on the sites
gluon fields, $A^a_\mu(x)$ are used as links and plaquettes

$$U(x, y) = \exp\left(ig_s \int_x^y dx'^\mu A^a_\mu(x')\lambda_a/2\right)$$

$$P_{\mu\nu}(n) = U_\mu(n)U_\nu(n + e_\mu)U^\dagger_\mu(n + e_\nu)U^\dagger_\nu(n)$$

$S = S_g + S_f$ consists of the pure gluonic and the fermionic parts

$$S_g = 6/g_s^2 \cdot \sum_{n,\mu,\nu} \left[1 - \mathrm{Re}(P_{\mu\nu}(n))\right]$$

# Lattice Lagrangian: fermionic fields

quark differencing scheme:

$$\bar{\psi}(x)\gamma^{\mu}\partial_{\mu}\psi(x) \rightarrow \bar{\psi}_n\gamma^{\mu}(\psi_{n+e_{\mu}} - \psi_{n-e_{\mu}})$$

$$\bar{\psi}(x)\gamma^{\mu}D_{\mu}\psi(x) \rightarrow \bar{\psi}_n\gamma^{\mu}U_{\mu}(n)\psi_{n+e_{\mu}} + ...$$

fermionic part as a bilinear expression: $S_f = \bar{\psi}_n M_{nm}\psi_m$
we need 2 light quarks (u,d) and the strange quark: $n_f = 2 + 1$

(complication: doubling of fermionic freedoms)

Euclidean partition function gives Boltzmann weights

$$Z = \int \prod_{n,\mu}[dU_{\mu}(x)][d\bar{\psi}_n][d\psi_n]e^{-S_g - S_f} = \int \prod_{n,\mu}[dU_{\mu}(n)]e^{-S_g}\det(M[U])$$

## Historical background

1972 Lagrangian of QCD (H. Fritzsch, M. Gell-Mann and H. Leutwyler)

1973 asymptotic freedom (D. Gross, F. Wilczek, D. Politzer)
  at small distances (large energies) the theory is "free"

1974 lattice formulation (Kenneth Wilson)
  at large distances the coupling is large: non-perturbative

Nobel Prize 2008: Y. Nambu, & M. Kobayashi T. Masakawa

spontaneous symmetry breaking in quantum field theory
  strong interaction picture: mass gap is the mass of the nucleon

mass eigenstates and weak eigenstates are different

**Z. Fodor**     **Ab initio calculations in lattice QCD**

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Scientific Background on the Nobel Prize in Physics 2008

"Even though QCD is the correct theory for the strong interactions, it can not be used to compute at all energy and momentum scales. For many purposes, the original idea, ... breaking of the ... symmetry of QCD, ... allows us to study the low energy dynamics of QCD, a region where perturbative methods do not work for QCD."

true, but the situation is somewhat better: new era
fully controlled non-perturbative approach works (took 35 years)

## Importance sampling

$$Z = \int \prod_{n,\mu} [dU_\mu(n)] e^{-S_g} \det(M[U])$$

we do not take into account all possible gauge configuration

each of them is generated with a probability $\propto$ its weight

Metropolis step for importance sampling:
(all other algorithms are based on importance sampling)

$$P(U \to U') = \min \left[1, \exp(-\Delta S_g) \det(M[U'])/\det(M[U])\right]$$

gauge part: trace of 3×3 matrices (easy, without M: quenched)
fermionic part: determinant of $10^6 \times 10^6$ sparse matrices (hard)

more efficient ways than direct evaluation (Mx=a), but still hard

# Hadron spectroscopy in lattice QCD

Determine the transition amplitude between:
having a "particle" at time 0 and the same "particle" at time t
$\Rightarrow$ Euclidean correlation function of a composite operator $\mathcal{O}$:

$$C(t) = \langle 0|\mathcal{O}(t)\mathcal{O}^\dagger(0)|0\rangle$$

insert a complete set of eigenvectors $|i\rangle$

$$= \sum_i \langle 0|e^{Ht}\,\mathcal{O}(0)\,e^{-Ht}|i\rangle\langle i|\mathcal{O}^\dagger(0)|0\rangle = \sum_i |\langle 0|\mathcal{O}^\dagger(0)|i\rangle|^2\,e^{-(E_i-E_0)t},$$

where $|i\rangle$: eigenvectors of the Hamiltonian with eigenvalue $E_i$.

and
$$\mathcal{O}(t) = e^{Ht}\,\mathcal{O}(0)\,e^{-Ht}.$$

$t$ large $\Rightarrow$ Lightest states (created by $\mathcal{O}$) dominate.
$t$ large $\Rightarrow$ Exponential fits or $M_{eff}$=log[C(t)/C(t+1)]

## Quenched results

properties of hadrons (Rosenfeld table) $\Rightarrow$ QCD is 35 years old

non-perturbative lattice formulation (Wilson) immediately appeared
needed 20 years even for quenched result of the spectrum (cheap)

always at the frontiers of computer technology:
GF11: IBM "to verify quantum chromodynamics" (10 Gflops, '92)
CP-PACS Japanese purpose made machine (Hitachi 614 Gflops, '96)
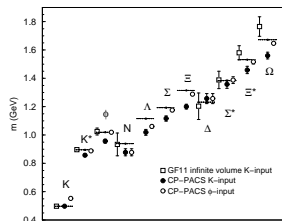


the $\approx$10% discrepancy was believed to be a quenching effect

## Difficulties of full dynamical calculations

though the quenched result is qualitatively correct
uncontrolled systematics $\Rightarrow$ full "dynamical" studies
by two-three orders of magnitude more expensive (balance)
present day machines offer several hundreds of Tflops

no revolution but evolution in the algorithmic developments
Berlin Wall '01: it is extremely difficult to reach small quark masses:



**Z. Fodor** **Ab initio calculations in lattice QCD**
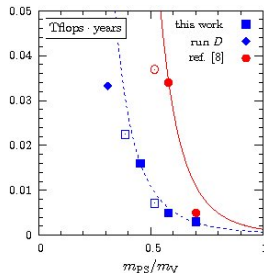
hadron masses (mass of the proton) many results in the literature

JLQCD, PACS-SC (Japan), MILC (USA), QCDSF (Germany-UK),
RBC & UKQCD (USA-UK), ETM (Europe), Alpha(Europe)
CERN-Rome (Swiss-Italian)

note, that all of them neglected one or more of the ingredients
required for controlling all systematics (it is quite CPU-demanding)

$\implies$ Budapest-Marseille-Wuppertal (BMW) Collaboration

new results, controlling all systematics: Science 322:1224-1227,2008
(F. Wilczek, Nature 456:449-450,2008)

http://www.bmw.uni-wuppertal.de

## Ingredients to control systematics

- inclusion of det[M] with an exact $n_f$=2+1 algorithm
  action: universality class is known to be QCD: Wilson-quarks
- spectrum for the light mesons, octet and decuplet baryons
  (three of these fix the averaged $m_{ud}$, $m_s$ and the cutoff)
- large volumes to guarantee small finite-size effects
  rule of thumb: $M_\pi L \gtrsim 4$ is usually used (correct for that)
- controlled interpolations & extrapolations to physical $m_s$ and $m_{ud}$
  (or eventually simulating directly at these masses)
  since $M_\pi \simeq 135$ MeV extrapolations for $m_{ud}$ are difficult
  CPU-intensive calculations with $M_\pi$ reaching down to $\approx$200 MeV
- controlled extrapolations to the continuum limit ($a \to 0$)
  calculations are performed at no less than 3 lattice spacings

# Action and algorithms

### action:
good balance between gauge (Symanzik improvement) and
fermionic improvements (clover and stout smearing) and CPU
gauge and fermion improvement with terms of $O(a^4)$ and $O(a^2)$

### algorithm:
rational hybrid Monte-Carlo algorithm with mass preconditioning
multiple time-scale integration, with Omelyan integrator and
mixed precision techniques

### parameter space:
series of $n_f$=2+1 simulations (degenerate $u$ and $d$ sea quarks)
separate $s$ sea quark, with $m_s$ at its approximate physical value
to interpolate: repeat some simulations with a slightly different $m_s$
we vary $m_{ud}$ in a range which corresponds to $M_\pi \approx$190—580 MeV
three different $\beta$-s, which give $a \approx$0.125 fm, 0.085 fm and 0.065 fm

## Further advantages of the action

smallest eigenvalue of M: small fluctuations
$\Rightarrow$ simulations are stable (major issue of Wilson fermions)

non-perturbative improvement coefficient: $\approx$ tree-level (smearing)

R. Hoffmann, A. Hasenfratz, S. Schaefer, PoS **LAT2007** (2007) 1 04

good $a^2$ scaling of hadron masses ($M_\pi/M_\rho$=2/3) up to $a\approx$0.2 fm

S. Dürr et al. [Budapest-Marseille-Wuppertal Collaboration] arXiv :0802.2706
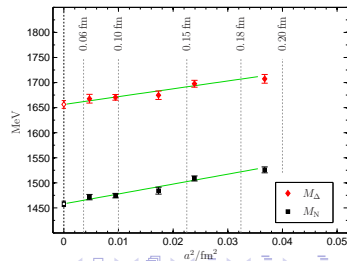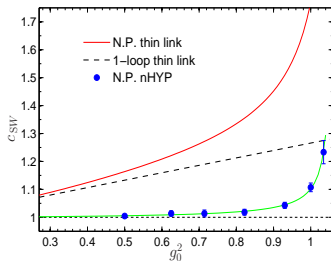
## Locality properties of the action

stout smearing 6 times: should we worry about locality (2 types)?
– in continuum the proper QCD action is recovered (ultra-local)
– does one receive at $a \neq 0$ unwanted contributions?

type A: $D(x, y)$=0 for all $(x, y)$ except for nearest neighbors
type B: dependence of $D(x, y)$ on $U_\mu$ at distance $z$
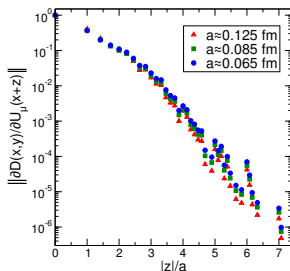


drops exponentially to $10^{-6}$ within the ultra-locality region: OK

masses are obtained by correlated fits (choice of fitting ranges)
illustration: effective masses at our smallest $M_\pi \approx 190$ MeV (noisiest)
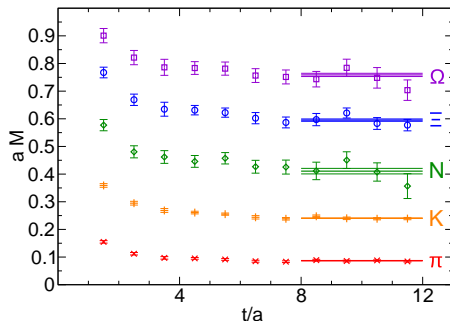


volumes and masses for unstable particles: avoided level crossing
decay phenomena included: in finite V shifts of the energy levels
$\Rightarrow$ decay width (coupling) & masses of the heavy and light states

## Parameters of the Lagrangian

three parameters of the Lagrangian: coupling strength $g$, $m_{ud}$ and $m_s$

asymptotic freedom: for large cutoff (small lattice spacing) $g$ is small
in this region the results are already independent of $g$ (scaling)

QCD predicts only dimensionless combinations (e.g. mass ratios)
$\Rightarrow$ we can eliminate $g$ as an input parameter by taking ratios

the pion mass $M_\pi$ is particularly sensitive to $m_{ud}$
the kaon mass $M_K$ is particularly sensitive to $m_s$

relatively easy to set the strange quark mass $m_s$ to its physical value
it is very CPU demanding to approach the physical $m_{ud}$

altogether 15 points for each hadrons
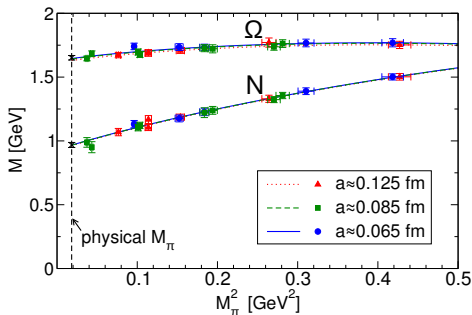


smooth extrapolation to the physical pion mass (or $m_{ud}$)
small discretization effects (three lines barely distinguishable)

continuum extrapolation goes as $c \cdot a^n$ and it depends on the action
in principle many ways to discretize (derivative by 2,3... points)
goal: have large $n$ and small $c$ (in our case $n = 2$ and $c$ is small)

## Final result for the hadron spectrum
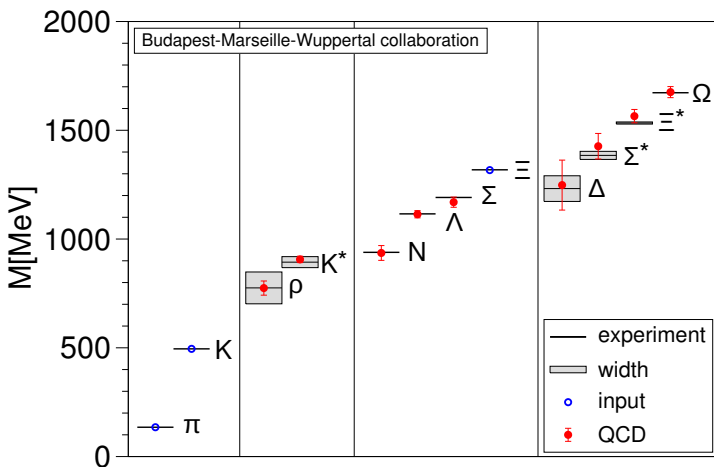
# Reality: smooth analytic transition (cross-over)
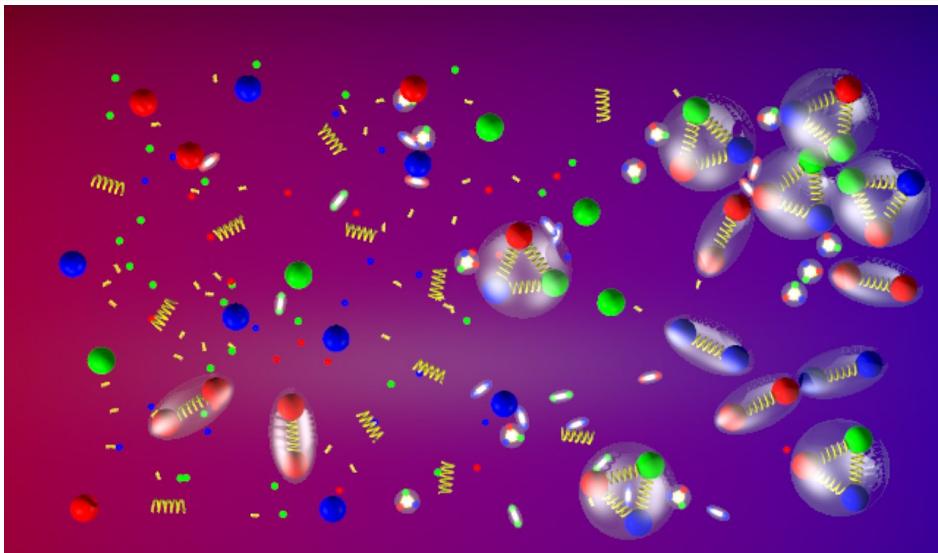
## Finite-size scaling theory

problem with phase transitions in Monte-Carlo studies
Monte-Carlo applications for pure gauge theories ($V = 24^3 \cdot 4$)
existence of a transition between confining and deconfining phases:
Polyakov loop exhibits rapid variation in a narrow range of $\beta$
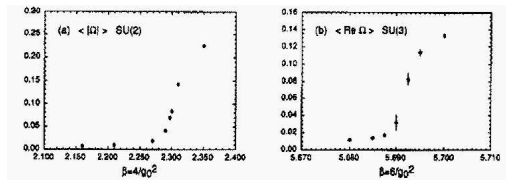


• theoretical prediction: SU(2) second order, SU(3) first order
$\implies$ Polyakov loop behavior: SU(2) singular power, SU(3) jump

data do not show such characteristics!

# Finite size scaling in the quenched theory

look at the susceptibility of the Polyakov-line
(trace of the product of the SU(3) matrices along the t-direction)
first order transition $\Longrightarrow$ peak width $\propto 1/V$, peak height $\propto V$
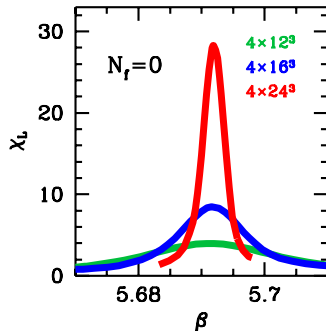


finite size scaling shows: the transition is of first order

## The nature of the QCD transition

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675

finite size scaling study of the chiral condensate (susceptibility)

$$\chi = (T/V)\partial^2 \log Z/\partial m^2$$

similar to the density of water (or to its derivative)
first order phase transition: density jumps (derivative divergent)
phase transition: finite V analyticity V$\to \infty$ increasingly singular
(e.g. first order phase transition: height $\propto$ V, width $\propto$ 1/V)
for an analytic cross-over $\chi$ does not grow with V

two steps (three volumes, four lattice spacings):
a. fix V and determine $\chi$ in the continuum limit: a=0.3,0.2,0.15,0.1fm
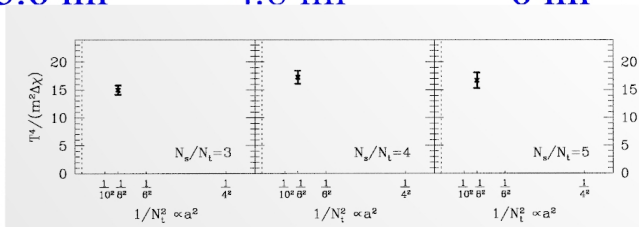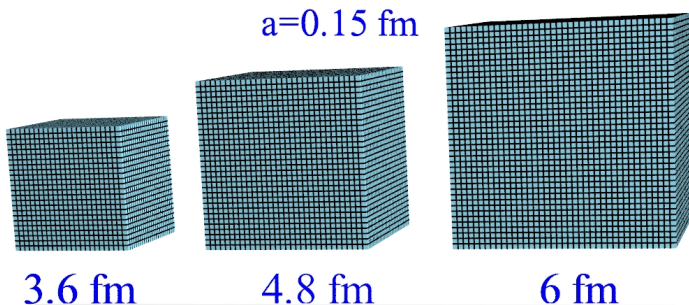b. using the continuum extrapolated $\chi_{max}$: finite size scaling

# Approaching the continuum limuit
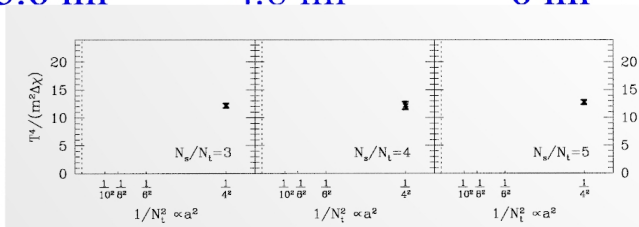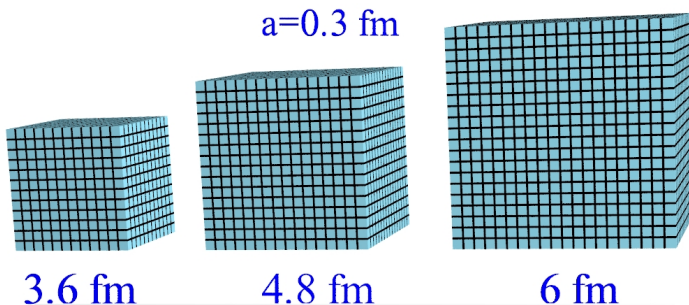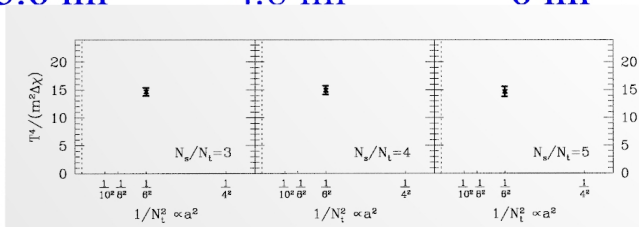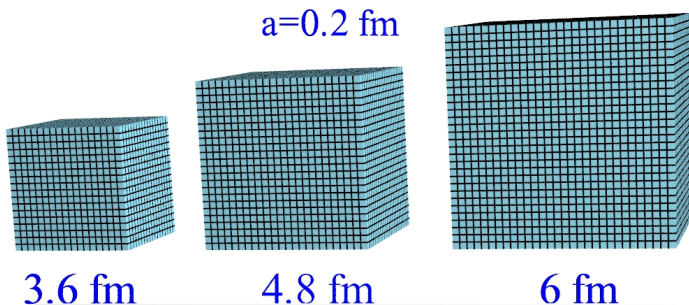
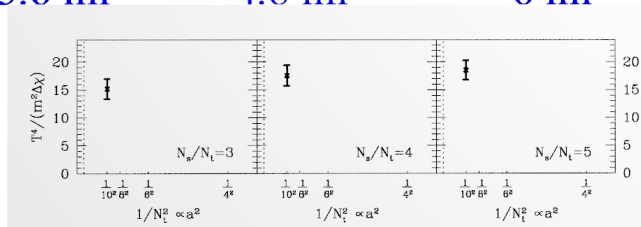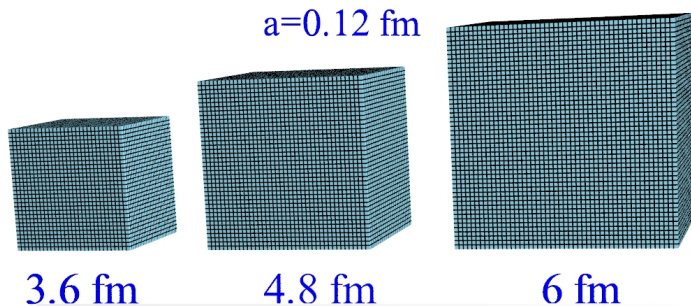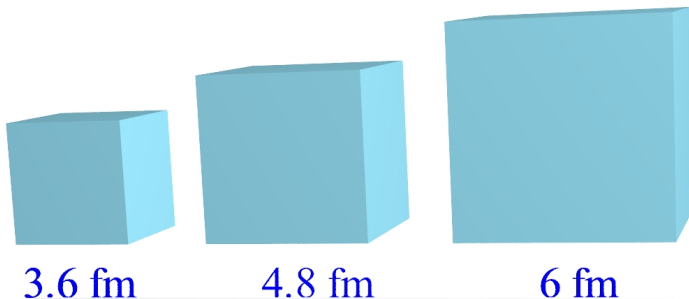# Approaching the continuum limuit



a=0.2 fm

3.6 fm          4.8 fm          6 fm

# Approaching the continuum limuit

# Approaching the continuum limuit



a=0.12 fm

3.6 fm          4.8 fm              6 fm

# Approaching the continuum limuit



3.6 fm          4.8 fm          6 fm
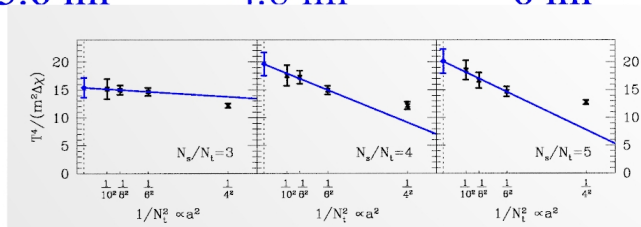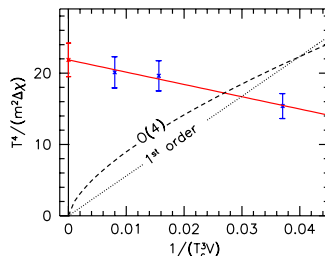
# The nature of the QCD transition: result

• finite size scaling analysis with continuum extrapolated m$^2 \Delta \chi / T^4$



the result is consistent with an approximately constant behavior
for a factor of 5 difference within the volume range
chance probability for 1/V is $10^{-19}$ for O(4) is $7 \cdot 10^{-13}$
continuum result with physical quark masses in staggered QCD:

the QCD transition is a cross-over

## The transition temperature

Y. Aoki, Z. Fodor, S.D. Katz, K.K. Szabo, Phys. Lett. B. 643 (2006) 46

an analytic transition (cross-over) has no unique $T_c$:
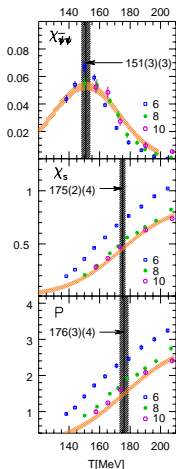example of water-steam transition
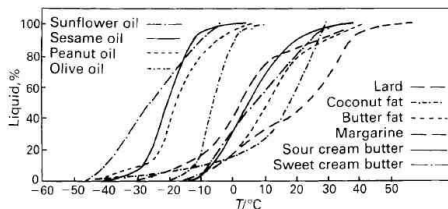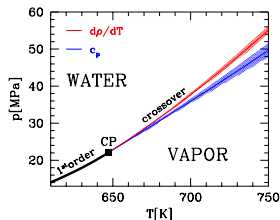


above the critical point $c_p$ and $d\rho/dT$ give different $T_c$s.
QCD: chiral & quark number susceptibilities or Polyakov loop
they result in different $T_c$ values $\Rightarrow$ physical difference

## The transition temperature: results and scaling



Chiral susceptibility
$T_c$=151(3)(3) MeV
$\Delta T_c$=28(5)(1) MeV

Quark number susceptibility
$T_c$=175(2)(4) MeV
$\Delta T_c$=42(4)(1) MeV

Polyakov loop
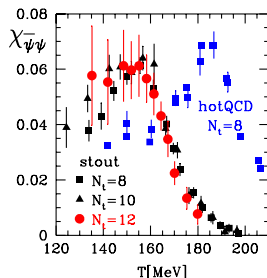$T_c$=176(2)(4) MeV
$\Delta T_c$=38(5)(1) MeV

$N_t$=6,8,10 in the $a^2$ scaling region, $N_t$=8,10(12) are practically the same

# Discrepancy between HotQCD and us

renormalized chiral susceptibility $m^2 \chi_{\bar\psi\psi}/T^4$



nice agreement with old $N_t = 8, 10$ data

Y. Aoki, Z. Fodor, S.D. Katz, K.K. Szabo, Phys. Lett. B 643 (2006) 46 [hep-lat/0609068]

"the transition temperature based on the chiral susceptibility reads $T_c(\chi_{\bar\psi\psi}) = 151(3)(3)$ MeV"

## Summary

- understanding the source and the course of the mass generation of ordinary matter is of fundamental importance

- after 35 years of work these questions can be answered (cumulative improvements of algorithms and machines are huge)

- they belong to the largest computational projects on record

- perfect tool to understand hadronic processes (strong interaction)

1. how is the mass of ordinary matter generated (what is its source)

- more than 99.9% of the mass of the visible universe is made up from protons and neutrons (ordinary matter)
  95% of the mass of a proton comes from the kinetic energy within the proton: very different from any other mass
- the standard model of particle physics (most particularly the theory of strong interaction, QCD) can explain this phenomena
- full ab-initio calculation of the masses
  (controlling all systematic uncertainties) ⇒ resonances' widths

2. how was the mass of ordinary matter generated (early universe)

- transition between the low temperature phase (dominated by color-neutrtal hadrons) and the high temperature phase (dominated by colored objects) ⇒ heavy ion collisions
- though these two phases are fundamentally different there is no singularity, just an analytic cross-over ⇒ phase diagram, $T_c$